

Carbamic acid, ethyl-, methyl ester
6135-31-5 | DTXSID80210261

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.68 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.00e-01

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl chloroacetate</div> <div>Measured: 9.05e-01</div> <div>Predicted: 7.43</div>	<div>Image not found</div> <div>Ethyl isobutyrate</div> <div>Measured: 3.75</div> <div>Predicted: 19.3</div>	<div>Image not found</div> <div>Tetradecylbenzene</div> <div>Measured: 1.70</div> <div>Predicted: 1.52e-05</div>
<div>Image not found</div> <div>2-Butenoic acid</div> <div>Measured: 12.5</div> <div>Predicted: 2.74e-01</div>	<div>Image not found</div> <div>Pirimicarb</div> <div>Measured: 1.30</div> <div>Predicted: 5.21e-06</div>	